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On the nature of the large- q expansion of the response for a non-relativistic confined systemE. Pace¹, G. Salmè²

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Abstract:

We show the equivalence of a previously derived exact expression for the response of a non-relativistic system with harmonic forces and an infinite sum of weighted δ -functions corresponding to the spectrum. We forward arguments, indicating that the Gersch-Rodriguez-Smith $1/q$ -expansion of the response does not converge and prove that this expansion is an asymptotic series.

In recent years there has been renewed interest in work by Gersch, Rodriguez and Smith (GRS). Those authors formally derived for large momentum transfer q , a $1/q$ expansion of the dominant incoherent part of the total non-relativistic (NR) response, $S(q, \omega)$, which is non-perturbative in V ¹. This approach has recently been applied, even if the underlying forces are singular and attractive (i.e. confining)². The incoherent part of the total reduced response $\phi(q, y) = (q/m)S(q, \omega) = \phi^{incoh}(q, y) + \phi^{coh}(q, y)$ may thus be expressed as

$$\phi^{incoh}(q, y) = \sum_{k=0}^{\infty} (m/q)^k F_k(y), \quad (1)$$

where the energy loss ω has been replaced by an alternative variable

$$y = -q/2 + m\omega/q \quad (2)$$

Up to now a detailed analysis of the convergence of GRS expansion of the response for NR systems, interacting either by regular or confining forces, is lacking. In the present note we consider the possibility that, even if this series does not converge, a finite number of terms may still describe the response at high q to any desired accuracy, as is the case for an asymptotic series.

Without reference to specific NR dynamics we consider the following three equivalent forms for the response of a target of mass m_A , composed of A constituents with equal mass m

$$S(q, \omega) = A^{-1} \sum_n |\mathcal{F}_{0n}(q)|^2 \delta(\omega - q^2/2m_A - E_{n0}) \quad (3a)$$

$$= (\pi A)^{-1} \langle 0 | \rho_q^\dagger \text{Im}(\omega + E_0 - T - V - i\eta)^{-1} \rho_q | 0 \rangle \quad (3b)$$

$$= (2\pi A)^{-1} (m/q) \int_{-\infty}^{\infty} ds e^{isy} e^{isq/2} \langle 0 | \rho_q^\dagger \exp \left[\frac{ism}{q} (E_0 - H) \right] \rho_q | 0 \rangle, \quad (3c)$$

where $\mathcal{F}_{0n}(q) = \langle 0 | \rho_q^\dagger | n \rangle$ is the inelastic form factor between the ground state $|0\rangle$ and excited states $|n\rangle$, E_{n0} are intrinsic excitation energies without the target recoil energy $q^2/2M_A$, which

appears separately in the energy conserving δ function in (3a), and ρ_q is the Fourier transform of the charge density. A formal summation over the excited states in (3a) produces (3b) in terms of the Green's function with T , V the total kinetic and potential energy. Eq. (3c) is the Fourier transform of (3b) and $H = T + V$ the total Hamiltonian of the system. Clearly it is meaningful only in the distribution theory.

We now concentrate on systems with confining interactions and shall be led to questions of equivalence of the different expressions (3). We shall illustrate our reasoning on the example of harmonic confining forces, for which an exact solution for the response in terms of a single integration has recently been derived³. It suffices to treat the case of two particles in a HO well. With $\beta = (m\Omega/2)^{1/2}$ the inverse oscillator length and $\alpha = 2\beta^2 s/q$ one finds for the reduced response

$$\phi^{incoh}(q, y) = \int_{-\infty}^{\infty} \frac{ds}{2\pi} \exp(iys) \Phi(\alpha, s) \quad (4a)$$

$$\phi^{coh}(q, y) = \int_{-\infty}^{\infty} \frac{ds}{2\pi} \exp(iys) \exp\left\{-\frac{\beta^2 s^2}{4} \left(\frac{\cos\alpha/2}{\alpha/2}\right)^2\right\} \exp\left\{iqs/4 \left(\frac{\sin\alpha}{\alpha} + 1\right)\right\} \quad (4b)$$

with

$$\Phi(\alpha, s) = \exp\left\{-\frac{\beta^2 s^2}{4} \left(\frac{\sin\alpha/2}{\alpha/2}\right)^2\right\} \exp\left\{-i\frac{\beta^2 s^2}{2\alpha} \left(\frac{\sin\alpha}{\alpha} - 1\right)\right\} \quad (5)$$

The exponents in Eq. (5) are readily seen to be sums of power series in α and thus permit an expansion of $\Phi(\alpha, s)$ in series of $1/q$, except for $q = 0$

$$\Phi(\alpha, s) = 2\pi \sum_{k=0}^{\infty} (1/q)^k h_k(s) \quad (6)$$

When permitted, interchange of summation and term by term integration leads to the GRS sum (1). The HO example is particularly useful for the discussion of two points:

1) With a priori knowledge of the equivalence of the expressions (3), can one directly demonstrate that the integrands in Eqs. (4), analytic except for $q = 0$, lead to a weighted sum of δ -functions?

2) The GRS expansion is formally generated through term by term integration of Eq. (4a) and it consists of a series of regular functions, (cf. Ref. 3, Eq. (3.1)). The sequence of the partial sums of this expansion does not seem to tend to a series of equally spaced peaks, required to obtain in the limit Eq. (3a), i.e. a sum of weighted, equally spaced δ -functions. In view of this unlikely equivalence, what is the nature of the GRS series (1)?

We start with the first point and rewrite (4a)

$$\begin{aligned}\phi^{incoh}(q, y) &= \exp(-q^2/8\beta^2) \int_{-\infty}^{\infty} \frac{ds}{2\pi} \exp(iys) \exp(iqs/4) D(q, s) \\ D(q, s) &= \exp\left[\frac{q^2}{8\beta^2} e^{-2i\beta^2 s/q}\right]\end{aligned}\tag{7}$$

The function $D(q, s)$ is periodic in $2\beta^2 s/q$ and thus permits the Fourier expansion

$$D(q, s) = \sum_{n=-\infty}^{+\infty} d_n(q, \beta) e^{-2in\beta^2 s/q}\tag{8}$$

with expansion coefficients

$$d_n(q, \beta) = \frac{2\beta^2}{q} \int_0^{\pi q/\beta^2} \frac{ds}{2\pi} e^{2in\beta^2 s/q} D(q, s) = \frac{1}{2\pi i} \left(\frac{q^2}{8\beta^2}\right)^n \xi_{n+1},\tag{9}$$

and

$$\xi_{n+1} \equiv (-1)^n \int dz z^{-(n+1)} e^{-z} = \frac{2\pi i}{n!}.\tag{10}$$

The integration in Eq. (10) is performed on a circle centered in the origin and of radius $|c| = q^2/8\beta^2$. Eq. (9) can be readily obtained from Eq. (10) with the substitutions $z = ce^{-i\alpha}$ ($2\pi \geq \alpha \geq 0$) and $c = -q^2/8\beta^2$.

In order to show the equivalence of Eqs. (3a) and (3c), we recall that Eqs. (3c), (4a) and (7) have meaning only in the framework of distributions. There we need the notion of ‘good’ functions $g(y)$, i.e. functions which are everywhere differentiable any number of times, and which together with their derivatives vanish as $|y| \rightarrow \infty$ faster than any power of $1/|y|^{4a}$. For any such g , Eq. (7) implies

$$\int_{-\infty}^{\infty} \phi^{incoh}(q, y) g(y) dy = (2\pi)^{-1} \exp(-q^2/8\beta^2) \int_{-\infty}^{\infty} e^{isq/4} D(q, s) \hat{g}(s) ds,\tag{11}$$

where $\widehat{g}(s)$ is the Fourier transform of $g(y)$. We note moreover

$$\left| \sum_{n=-N}^N d_n(q, \beta) e^{-2in\beta^2 s/q} \right| \leq \sum_{n=-N}^N \left(\frac{q^2}{8\beta^2} \right)^n \frac{1}{n!} \leq 2 e^{(q^2/8\beta^2)} \quad (12)$$

and that the right hand side of Eq. (12) is independent of N . The Lebesgue dominated convergence theorem ^{4b} then permits inversion of the order of integration and summation of the series in Eq. (7) and one readily finds

$$\begin{aligned} S^{incoh}(q, \omega) &= \frac{m}{q} e^{-(q^2/8\beta^2)} \sum_{n=-\infty}^{+\infty} \frac{1}{n!} \left[\frac{q^2}{8\beta^2} \right]^n \delta(\omega - q^2/4m - n\Omega) \\ &= e^{-(q^2/8\beta^2)} \sum_{n=0}^{+\infty} \frac{1}{n!} \left[\frac{q^2}{8\beta^2} \right]^n \delta[y + q/4 - (2\beta^2 n/q)] \end{aligned} \quad (13)$$

A similar expression can be derived for the coherent part and one checks that the weights of the δ -functions are the exact squared inelastic form factors for the HO⁵. Notice that for $\omega > 0$, only $n \geq 0$, i.e. the actual HO spectrum, contributes to (13).

In spite of its utter simplicity, the above explicit demonstration of equivalence is not trivial at all, nor does it serve as a model for other confining interactions. Only for a very limited number of Hamiltonians can one give closed forms for the exact response, using either exact Green's function⁶ or operator techniques³. In addition, for no other interaction can the corresponding function $D(q, s)$ in (8) be periodic: it would lead to an equally spaced spectrum, characteristic for the HO. In general a regular Hamiltonian has a finite number of unequally spaced discrete eigenvalues. In any case the proof above for the equivalence of Eqs.(3a) and (3c) is not readily seen to be of a general type.

We return to Eq. (4a). We already observed that the integrand in Eq. (4a) permits a $1/q$ -expansion, which produces the GRS series if the order of summation and integration may be interchanged. However, we have not been able to prove a condition like Eq. (12) for the partial sum of the power expansion of $\Phi(\alpha, s)$, Eq. (6). A *finite* number of terms in the $1/q$ expansion may always be integrated term by term, thus leading to a truncated GRS series and this has been standard practice for systems with regular interactions. A prime

example is the successful treatment of liquid ^4He ⁷. However, the crucial question is whether the above interchange is permitted for the *full* series. If the GRS series does not converge, it may still be an asymptotic one ⁸ and we now show that this is the case for the HO.

Consider the sequence $\{S_n(q, y)\}$

$$S_n(q, y) = \sum_{k=0}^n (1/q)^k \int_{-\infty}^{+\infty} h_k(s) e^{iys} ds. \quad (14)$$

All integrals in Eq. (14) are well defined, since $h_k(s)$ is a linear combination of powers of s times $\exp(-\beta^2 s^2/4)$ and therefore $h_k(s) \in \mathcal{L}^1$. We wish to show that the sequence $\{S_n(q, y)\}$ defines an asymptotic series for $\phi^{incoh}(q, y)$. To this end we have to show that for any fixed n and any good function $g(y)$, for any given $\epsilon > 0$ a $Q > 0$ exists such that, for $q > Q$ one has $A_n(q) \leq \epsilon^{4a}$ with

$$\begin{aligned} A_n(q) &= q^n \left| \int_{-\infty}^{+\infty} \phi^{incoh}(q, y) g(y) dy - \int_{-\infty}^{+\infty} S_n(q, y) g(y) dy \right| \\ &= q^n \left| \int_{-\infty}^{+\infty} \sum_{k=0}^{\infty} (1/q)^k h_k(s) \hat{g}(s) ds - \int_{-\infty}^{+\infty} \sum_{k=0}^n (1/q)^k h_k(s) \hat{g}(s) ds \right| \end{aligned} \quad (15)$$

In the second term of the last step of Eq. (15) the order of integrations has been exchanged by using the Fubini theorem^{4b}. Eq. (15) can be put in the following form

$$A_n(q) = \frac{1}{q} \left| \int_{-\infty}^{+\infty} \frac{1}{(n+1)!} \Phi^{(n+1)}(\alpha_o, s) \hat{g}(s) ds \right|, \quad (16)$$

where $\Phi^{(n+1)}(\alpha, s) \equiv (\partial/\partial x)^{(n+1)} \Phi(\alpha, s)$, $x = 1/q = \alpha/(2\beta^2 s)$, and $\alpha_o = 2\beta^2 s/q_o$ with $q_o > q$. If one can show that for any $\alpha \in (-\infty, +\infty)$

$$\left| \Phi^{(n+1)}(\alpha, s) \right| \leq \mathcal{P}_{(n+1)}(s), \quad (17)$$

with $\mathcal{P}_{(n+1)}(s)$ diverging at most as a power of s , our theorem is demonstrated. It is easily seen that the derivative $\Phi^{(n+1)}(\alpha, s)$ is a product of $\Phi(\alpha, s)$ and combinations of ℓ -th order derivatives ($\ell \leq n+1$) of $a(\alpha) = \sin(\alpha/2)/(\alpha/2)$ and $b(\alpha) = (\sin\alpha/\alpha - 1)/\alpha$ with respect to α , with coefficients depending on powers of s with bounded exponents for a given n .

We thus have to study the behaviour of $a(\alpha)$, $b(\alpha)$ and their derivatives for $\alpha \in (-\infty, +\infty)$. Consider separately the two sets $|\alpha| \leq 1$ and $|\alpha| > 1$. In the range $[-1, 1]$ one may expand $a(\alpha)$ and $b(\alpha)$ as a power series in α , which together with the series defining their derivatives, converge uniformly in the closed set $[-1, 1]$ and their absolute values have there finite maxima. For $|\alpha| > 1$, the functions $a(\alpha)$, $b(\alpha)$ and their derivatives can be expressed as combinations of $\sin\alpha$, $\cos\alpha$ and powers of $1/|\alpha| < 1$. One can therefore find quantities, independent of α , which are larger than the absolute values of $a(\alpha)$, $b(\alpha)$ and their derivatives for any $\alpha \in (-\infty, +\infty)$. Consequently (17) holds and our theorem is demonstrated.

We summarize: Although the GRS expansion for the response of NR systems turns out to be a useful tool, we are not aware of an actual proof that the above expansion for systems, interacting through regular or confining forces is a convergent, or at least an asymptotic one. In this note we have proved that the latter is the case for the $1/q$ -expansion of the response for an harmonic oscillator.

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